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## Nomenclature

$\alpha$	Relative occupancy
$\chi$	Non-diffusive numerical tracer
$\dot{\gamma}$	Shear rate, $\text{s}^{-1}$
$\text{Co}$	Courant number
$\mu$	Power-law viscosity, $\text{Pa s}$
$\tau$	Shear stress, $\text{Pa}$
$\tau_0$	Herschel-Bulkley critical shear stress, $\text{Pa}$
$\mathbf{u}$	Liquid phase velocity field, $\text{m s}^{-1}$
$\Xi$	Rectangular function
$I$	Tracer concentration interval
$K$	Power-law consistency coefficient, $\text{Pa s}^n$
$n$	Power-law index
$t$	Time, $\text{s}$
$V$	Volume, $\text{m}^3$
CFD	Computational Fluid Dynamics
GCI	Grid Convergence Index
UI	Uniformity Index

## 1. Introduction

10 The wastewater industry is expected to face unprecedented pressures in the forthcoming  
 11 decades. The worldwide demand for clean water is growing, with 50% more food and 30%  
 12 more water needed by 2030 (WWAP (World Water Assessment Programme), 2012). In  
 13 addition, tightening EU regulations (specifically, the Water Framework Directive, WFD)  
 14 will cause wastewater treatment works (WwTWs) to increase energy consumption by up to  
 15 60% in the next 10-15 years (European Environment Agency, 2015). The need to mitigate

16 and adapt to climate change imposes renewed efforts towards energy efficiency and energy  
17 reuse, and hence it is clear that the link between wastewater and energy must be addressed  
18 (Dapelo and Bridgeman, 2018).

19 In 2010-2011, WwTWs in the UK produced 1.5M tonnes of municipal sewage sludge, the  
20 by-product of wastewater treatment (WaterUK, 2012). Sludge is often treated using  
21 mesophilic anaerobic digestion in which it is mixed with anaerobic bacteria at temperatures  
22 between 22 and 41°C. As biodegradable material is broken down into more stable  
23 compounds, a methane-rich biogas is produced and subsequently harnessed as a renewable  
24 energy via combined heat and power technology. Although mixing is responsible for  
25 17–73% of the energy consumption of an industrial digester (Owen, 1982), current practice  
26 in digester design is still rooted in rules of thumb and empiricism rather than science  
27 (Dapelo et al., 2015). Therefore, there is an urgent need to revise the way mixing is designed  
28 and operated within industrial digesters in order to improve the balance between input  
29 mixing energy and biogas output—i.e. to reduce input mixing power without compromising,  
30 and indeed enhancing, biogas yield. (Dapelo and Bridgeman, 2018). Recent experimental  
31 evidence (Kress et al., 2018) shows that it is possible to halve input mixing power without  
32 impacting nutrient distribution.

33 Computational fluid dynamics (CFD) is a powerful tool that can be used to study flow  
34 patterns of non-Newtonian sludge and mixing (Vesvikar and Al-Dahhan, 2005; Karim et al.,  
35 2007; Meroney and Colorado, 2009; Terashima et al., 2009; Wu, 2010; Bridgeman, 2012;  
36 Sindall et al., 2013; Craig et al., 2013; Dapelo et al., 2015; Hurtado et al., 2015; Zhang et al.,  
37 2016; Dapelo and Bridgeman, 2018; Lebranchu et al., 2017; Meister et al., 2018). However,  
38 the work undertaken so far is limited. First of all, whilst biogas mixing, both confined (i.e.,  
39 biogas injection performed inside an internal draft tube) and unconfined (i.e., without  
40 internal draft tube), is commonplace (despite not being the most efficient way of mixing:  
41 Brade and Noone 1981; Wu 2010) as the lack of moving elements inside digesters reduces

42 wear and maintenance, the amount of literature dedicated to it is still very limited when  
43 compared to other forms of mixing. Only Vesvikar and Al-Dahhan (2005); Wu (2010,  
44 2012b, 2014); Dapelo et al. (2015); Dapelo and Bridgeman (2018) have proposed robust  
45 multiphase models and only Wu (2010, 2012b, 2014); Dapelo and Bridgeman (2018) have  
46 considered full-scale digesters.

47 Another limitation of CFD work undertaken to date is the lack of a clear criterion to assess  
48 mixing quality. Camp and Stein (1943) proposed the average shear rate as the fundamental  
49 process characteristic to classify mixing in vessels, and the water industry traditionally  
50 adopts the approach of considering digester mixing as satisfactory when the average shear  
51 rate exceeds  $50\text{--}80\text{ s}^{-1}$  (Tchobanoglous et al., 2010). However, this criterion has been  
52 shown to be inadequate for the case of sludge mixing for anaerobic digestion. Previous  
53 laboratory-based and full-scale work has demonstrated that anaerobic digestion takes place  
54 under a much lower average shear rate—up to one order of magnitude lower for  
55 laboratory-scale (Bridgeman, 2012; Sindall et al., 2013), and two orders of magnitude lower  
56 for full-scale (Dapelo and Bridgeman, 2018).

57 Furthermore, the approach of minimum average shear rate has been criticized on the basis  
58 that the representation of complex flow patterns through one number is something of an  
59 over-simplification (Clark, 1985), especially considering that, in a mixed tank, areas of high  
60 local shear rate and dead zones are likely to coexist (Bridgeman, 2012; Sindall et al., 2013;  
61 Dapelo et al., 2015). However, there is no universally-accepted alternative approach in the  
62 literature.

63 Meroney and Colorado (2009); Terashima et al. (2009); Hurtado et al. (2015) evaluated the  
64 mixing performance of different full-scale digesters through CFD simulations of tracer  
65 washout parameters (viz. turnover time and dead volume) and tracer response curve. This  
66 approach avoids costly and time-consuming fieldwork experiments and has the fundamental  
67 advantage of providing an evaluation of mixing quality before digester construction.

68 However, it only gives a “black box” representation of the flow through the digester (Dapelo  
69 and Bridgeman, 2018). Meroney and Colorado (2009); Hurtado et al. (2015) evaluated  
70 velocity, turbulence intensity and tracer flow patterns and passive Lagrangian particle  
71 distributions, but their analyses were limited to qualitative considerations.

72 Hurtado et al. (2015) followed Vesvikar and Al-Dahhan (2005) and defined the dead volume  
73 as the portion of domain where velocity magnitude was below 5% of the maximum velocity.  
74 However, this method does not constitute a comprehensive evaluation of mixing because the  
75 choice of the minimum threshold of 5% is arbitrary, and local variations of velocity  
76 magnitude may unrealistically alter the definition of dead zone. (Dapelo and Bridgeman,  
77 2018) followed the idea that higher shear rate values imply better mixing. However, instead  
78 of providing a simple average figure as in Tchobanoglous et al. (2010), local shear values  
79 were used to identify very low, low, average and high shear rate zones within the  
80 computational domain, and the volume ratio of such zones over the whole volume were  
81 compared to each other in order to assess mixing quality. This method was successful in  
82 ascertaining that the digester design considered was subject to over-mixing. However, the  
83 approach provided only comparative data, and failed to provide information when mixing  
84 was time-dependent (i.e., when biogas injection was switched between two different nozzle  
85 series).

86 To date, the only attempt to introduce a quantitative, unequivocal criterion for mixing  
87 quality that takes into account the complexity of the flow patterns within a closed tank is that  
88 of Terashima et al. (2009). A non-diffusive tracer was defined throughout the computational  
89 domain, and the uniformity index (UI) was defined as the tracer’s absolute relative mean  
90 deviation. UI was used to assess different impeller mixing regimes and sludge total solid  
91 (TS) contents. However, Terashima et al. (2009) considered only draft-tube impeller mixing,  
92 and the analysis incorporated a number of limitations, including a limitation on  
93 time-independent mixing, and application only to laminar flow.

94 To address the lack of biogas-mixed anaerobic digestion CFD modelling, a two-phase  
95 Euler-Lagrangian model was developed and validated against lab-scale experimental data  
96 (Dapelo et al., 2015; Sindall et al., 2017). Dapelo and Bridgeman (2018), explained the  
97 difficulty of validating CFD models involving opaque sludge, and proposed a two-fold  
98 approach of a lab-scale validation of the model (which was performed in (Dapelo et al.,  
99 2015; Sindall et al., 2017), and applying the validated data to a set of full-scale scenarios.  
100 The inherent advantages of the Euler-Lagrangian formulation over other two-phase models  
101 have been explained elsewhere (Dapelo et al., 2015; Dapelo and Bridgeman, 2018). In  
102 addition to the above-mentioned evaluation of mixing through shear rate relative occupancy  
103 assessment, a full-scale application of the model (Dapelo and Bridgeman, 2018) showed for  
104 the first time the potential beneficial effect of time-dependent mixing—in particular,  
105 switching biogas injection between two different nozzle series at regular time intervals was  
106 shown to counter viscosity-driven short-circuiting, and greatly improved the spread of a  
107 numerical, non-diffusive scalar tracer. However, the mixing criterion based on shear rate  
108 relative occupancy evaluation failed to provide quantitative information.

109 Within the work described in this paper, a comprehensive set of different biogas-mixing  
110 methods for full-scale anaerobic digestion, including time-dependent mixing, are  
111 quantitatively assessed and compared for the first time in terms of mixing efficiency. Dead  
112 volume and uniformity index are assessed, and their suitability to produce practical results  
113 evaluated for the first time. In addition, a novel qualitative method is proposed to analyze  
114 the mixing conditions and the behaviour of a digester over time. A numerical tracer is  
115 defined as a scalar tracer obeying the non-diffusive advection-diffusion equation, different  
116 (logarithmic) intervals for concentration value defined, and the relative occupancy of each  
117 interval is evaluated. The results demonstrate that this method provides useful information

on mixed and unmixed areas within the digester.

## 2. Materials and Methods

### 2.1. Assessment of Mixing

Mixing is assessed through the introduction of a numerical tracer. Numerically, the tracer's concentration is described through a scalar field obeying a non-diffusive advection-diffusion equation:

$$\partial_t \chi + (\mathbf{u} \cdot \nabla) \chi = 0 , \quad (1)$$

where  $\chi$  is the tracer concentration, and  $\mathbf{u}$  is the velocity vector field. At the initial timestep ( $t = 0$ ), the tracer is seeded into different points of the digester. Numerically, this means that  $\chi$  is initialized as  $\chi = 1$  in small, localized portions of the computational domain, and as  $\chi = 0$  elsewhere. The distribution of the scalar field  $\chi(\mathbf{x})$  at the subsequent timesteps is used to assess mixing quality, as described in the following Sections.

#### 2.1.1. Uniformity Index

The uniformity index (UI) is defined following Terashima et al. (2009). Let  $V_i$  be the volume of the  $i$ -th cell in the computational domain, and  $\chi_i$  the (discretized) value of  $\chi$  therein. The total volume of the computational domain  $V$  and the average tracer concentration  $\bar{\chi}$  are:

$$V = \sum_i V_i , \quad (2)$$

$$\bar{\chi} = \frac{1}{V} \sum_i V_i \chi_i . \quad (3)$$

The uniformity index is defined as:

$$\text{UI} := \frac{1}{2V\bar{\chi}} \sum_i |\chi_i - \bar{\chi}| V_i . \quad (4)$$

Following Terashima et al. (2009), it is straightforward to show that UI is bounded between



0 and 1, with  $\chi = 0$  indicating perfect uniformity, and  $\chi = 1$  total inhomogeneity, which means, numerically, the tracer being confined at the seeding locations only. For the case of perfect uniformity,  $\chi_i = \bar{\chi} \forall i$ , and hence:

$$UI_{\min} = \frac{1}{2V\bar{\chi}} \sum_i |\bar{\chi} - \bar{\chi}| V_i = 0 . \quad (5)$$

If the tracer is concentrated in a single cell  $s$ , we have  $\chi_s = V/V_s \bar{\chi}$ , and  $\chi_{i \neq s} = 0$ . Then:

$$\begin{aligned} UI_{\max} &= \frac{\left| \frac{V}{V_s} \bar{\chi} - \bar{\chi} \right| V_s}{2V\bar{\chi}} + \frac{1}{2V\bar{\chi}} \sum_{i \neq s} |0 - \bar{\chi}| V_i \\ &= \frac{(V - V_s) \bar{\chi}}{2V\bar{\chi}} + \frac{(V - V_s) \bar{\chi}}{2V\bar{\chi}} = \frac{V - V_s}{V} \simeq 1 \quad (V_s \ll V) . \end{aligned} \quad (6)$$

#### 2.1.2. Dead Volume

The dead volume criterion was first introduced by Vesvikar and Al-Dahhan (2005). Contrary to the UI case, this method is based on fluid velocity rather than tracer concentration: at a given time, the maximum fluid velocity within the system is measured, and the portion of the computational domain where the velocity magnitude is below 5% of the maximum velocity is labelled as dead volume.

Dead volume is considered as cut off from the surrounding flow patterns; consequently, new influent sludge is considered unable to reach dead volume, and anaerobic digestion is considered as not taking place there. As such, a primary objective of mixing consists of minimizing dead volume.

#### 2.1.3. Relative Occupancy of Concentration Intervals

The degree of uniformity of the tracer is assessed as follows. The interval of values  $I \equiv [0, 1]$  that  $\chi$  can assume is decomposed into  $N$  sub-intervals  $\{I_i\} \equiv I_1, \dots, I_N$  such

153 that  $I_i \cup \dots \cup I_N = I$ . For each sub-interval  $I_i$ , the relative occupancy  $\alpha_i$  is defined as:

$$\alpha_i := \frac{\int d^3x \Xi_i(\chi(\mathbf{x}))}{\int d^3x}, \quad i = 1, \dots, N, \quad (7)$$

154 where the rectangular functions  $\Xi_i(\chi)$  are defined as:

$$\Xi_i(\chi) := \begin{cases} 1, & \chi \in I_i; \\ 0, & \chi \notin I_i; \end{cases} \quad i = 1, \dots, N. \quad (8)$$

155 This definition implies that  $\sum_{i=1}^N \alpha_i = 1$ . When the tracer field  $\chi$  becomes uniform (and  
 156 hence, the system is well-mixed), one single occupancy  $\alpha_m$  becomes much larger than all  
 157 the others, regardless of its particular value, but excluding  $\alpha_1$ , where it was considered that  
 158  $I_i \ni \chi \equiv 0$ . In this latter case, in fact, the tracer has not been able to spread through the  
 159 domain, with  $\chi \simeq 1$  in the small seeding regions, and  $\chi \simeq 0$  in the rest of the domain.

160 Given two different system configurations, described by the two sets of relative occupancies  
 161  $\{\alpha_i\}$  and  $\{\beta_i\}$  respectively, both with the same sub-domain decomposition  $I_1, \dots, I_N$ , the  
 162 first configuration is considered as better mixed if  $\max_{i \neq 1} \alpha_i > \max_{j \neq 1} \beta_j$ .

## 163 2.2. CFD Modelling

164 Below, the basic assumptions in modelling biogas-mixed sludge are described—a detailed  
 165 description of the CFD model is reported elsewhere (Dapelo et al., 2015; Dapelo and  
 166 Bridgeman, 2018).

### 167 2.2.1. Liquid Phase

168 Sludge is a complex mixture of water, flocculant and sedimenting matter, and biogas  
 169 bubbles due to biogas mixing. Within this work, mixing was only considered from the  
 170 perspective of providing a homogeneous environment for bacteria, with nutrients being  
 171 spread evenly—the impact of mixing on sedimentation and flocculation prevention was

172 ignored at this stage. This choice was justified by the fact that flocculation and  
 173 sedimentation take place through time scales of days, if not years, whereas the simulations  
 174 performed within this work spanned a physical time of 20 minutes. Consequently, the liquid  
 175 and solid fractions were modelled together as a single continuous, constant-density liquid  
 176 phase obeying the incompressible Navier-Stokes equations.

### 177 2.2.2. *Rheology*

178 Sludge is known to have a complex rheology (Eshtiaghi et al., 2013), that is a function of  
 179 total solids content (TS), temperature (Achkari-Begdouri and Goodrich, 1992) and digestion  
 180 progress (Hreiz et al., 2017). Non-Newtonian behaviour been shown to affect fluid flow  
 181 patterns inside a digester (Wu and Chen, 2008) and consequently, non-Newtonian modelling  
 182 has become an important element of CFD modelling of anaerobic digestion.

183 The most common and straightforward model is the pseudoplastic (Terashima et al., 2009;  
 184 Wu, 2010, 2013; Bridgeman, 2012; Wu, 2014; Dapelo et al., 2015; Hurtado et al., 2015;  
 185 Zhang et al., 2016; Sindall et al., 2017; Dapelo and Bridgeman, 2018; Lebranchu et al.,  
 186 2017; Meister et al., 2018) in which apparent viscosity  $\mu$  and shear rate magnitude  $|\dot{\gamma}|$  obey  
 187 a power-law relationship:

$$\mu = K |\dot{\gamma}|^{n-1} , \quad (9)$$

188 where “pseudoplastic” means  $n < 1$ , and  $K$  is the consistency coefficient.

189 A more recent approach consists of using the Herschel-Bulkley model (Craig et al., 2013;  
 190 Hurtado et al., 2015; Dapelo and Bridgeman, 2018). Here, the power-law flow occurs only if  
 191 the shear stress exceeds a critical value  $\tau_0$ :

$$\mu = \tau_0 |\dot{\gamma}|^{-1} + K |\dot{\gamma}|^{n-1} . \quad (10)$$

192 In the work reported here, both the power-law (Eq. 9) and the Herschel-Bulkley model

(Eq. 10) were adopted, together with a Newtonian model for comparison. For the power-law model, data from Landry et al. (2004) was adopted for TS value of 2.5, 5.4 and 7.5%, while for the Herschel-Bulkley, data was taken from Baudez et al. (2013) for a TS value of 1.85%. These values were chosen in order to cover the range of the most common feeds for industrial digesters, and for comparison with previous work (Wu, 2010, 2012a; Bridgeman, 2012) and with previous validation and application of the CFD model used in this work (Dapelo et al., 2015; Dapelo and Bridgeman, 2018) and dependence on digestion progress was ignored because of the semi-continuous nature of the considered digesters. Table 1 reports the rheological models used in this work in numerical detail.

[Table 1 about here.]

As in Dapelo and Bridgeman (2018), the numerical solvers switched to a Newtonian model continuously when the local shear rate dropped below the user-defined threshold of  $0.001 \text{ s}^{-1}$  in order to avoid a singularity at  $|\dot{\gamma}| = 0$ . When appropriate, the relations described in Eq. 9 and 10 with the coefficients reported in Table 1 were extrapolated beyond the experimentally-measured range. Mesophilic anaerobic digestion maintains constant temperature conditions ( $35^\circ\text{C}$ ), and therefore sludge rheology's dependence on temperature (Baudez et al., 2013) was ignored. As discussed in Dapelo et al. (2015), the values of density for the TS range considered vary from  $1,000.36$  to  $1,001.73 \text{ kg m}^{-3}$  (Achkari-Begdouri and Goodrich, 1992), which differ for less than 1% from water density at 35 degrees ( $994 \text{ kg m}^{-3}$ ), and therefore density was approximated to  $1,000 \text{ kg m}^{-3}$  in all cases.

### 2.2.3. Bubble Phase & Multiphase Model

Mixing in biogas-mixed anaerobic digesters is driven by the rise of bubble plumes. This means that the faithful simulation of flow patterns throughout the computational domain requires robust modelling of the bubble-liquid phase momentum exchange, but the details of liquid phase motion around the bubbles are unimportant. A solution was proposed and

218 validated by Dapelo et al. (2015) and applied for the first time to full-scale design by Dapelo  
219 and Bridgeman (2018), and consisted of an Euler-Lagrangian multiphase CFD model, which  
220 was shown in the literature to be an effective balance between robustness, economy,  
221 flexibility and accuracy given the requirements described above. As described in  
222 Sections 2.2.1 and 2.2.2, the water-TS mixture was considered as a single, non-Newtonian  
223 liquid phase, while the gas phase was modelled as a bubble ensemble subjected to the  
224 following assumptions: (i) one bubble per parcel, (ii) spherical bubbles, and (iii) pointwise  
225 bubbles.

226 The inter-phase momentum exchange was modelled as a two-way coupling (liquid phase  
227 and single bubbles exchange momentum each other, but bubbles do not between  
228 themselves), this being justified by the observation in Dapelo et al. (2015); Dapelo and  
229 Bridgeman (2018) and in the simulations performed within this work, that the bubbles are  
230 always well-distanced from one another. Following Dapelo et al. (2015), the force acting on  
231 a bubble from the surrounding liquid phase (and, consequently, the same force with opposite  
232 sign, acting on the surrounding liquid phase from the bubble) consisted of the sum of  
233 buoyancy, drag as in Dewsbury et al. (1999) and lift as in Tomiyama et al. (2002). In order  
234 to compute the drag term correctly, the particle Reynolds number was determined locally,  
235 from the sum of liquid phase apparent and eddy viscosity.

236 Nominal bubble size is a required input data to compute inter-phase force, but no data are  
237 available in the literature on bubble diameter within anaerobic digesters. Dapelo and  
238 Bridgeman (2018) performed CFD simulations with three different bubble sizes (2, 6 and 10  
239 cm diameter), and showed that velocity and viscosity flow patterns were only marginally  
240 affected by the choice of the bubble size. Consequently, for this work, only the maximum  
241 bubble size considered in Dapelo and Bridgeman (2018) of  $d = 10$  cm was chosen in order  
242 to minimize the computational expense.

#### 243 2.2.4. *Meshing*

244 A cylindrical digester with an inclined base was simulated (Fig. 1).

245 [Figure 1 about here.]

246 In the first instance, a series of twelve nozzles, equally-spaced along a circle at the sloped  
 247 bottom of the tank was considered. A second series, with the nozzles placed along a  
 248 concentric circle of different diameter, was subsequently considered in an amended design  
 249 alongside the original one. The geometric details are reported in Table 2.

250 [Table 2 about here.]

251 The mesh consisted of a  $\pi/6$  radian wedge, with a single nozzle per nozzle series lying on  
 252 the symmetry plane of the wedge. Four grids were generated (Table 3).

253 [Table 3 about here.]

254 The computational work was undertaken using the BlueBEAR high performance computing  
 255 facility at the University of Birmingham. Each simulation was run in parallel on 12-core  
 256 Intel Xeon E5-2690 v3 Haswell sockets running at 2.6GHz with 128 GB RAM, for a total of  
 257 36 cores. OpenFOAM 2.3.0 with user-modified solver and libraries for the biogas phase,  
 258 was used to run the computational work. The computational runtime was between ten hours  
 259 and five days.

260 The turbulent motion of the liquid around the bubbles was modelled through the Reynolds  
 261 stress Launder-Gibson model (Gibson and Launder, 1978; Dapelo et al., 2015; Dapelo and  
 262 Bridgeman, 2018).

263 The timestep was defined dynamically as in Dapelo et al. (2015); Dapelo and Bridgeman  
 264 (2018), via computation of the maximum Courant number. For a given cell,  $i$ , of linear

265 magnitude  $L_i$  where the fluid velocity is  $|\mathbf{u}_i|$ , given the timestep  $\Delta t$ , the Courant number is  
 266 defined as:

$$\text{Co}_i = \frac{|\mathbf{u}_i| \Delta t}{L_i} . \quad (11)$$

267 The maximum Courant number,  $\text{Co}$ , is the maximum value of  $\text{Co}_i$  over  $i$ . Following Dapelo  
 268 et al. (2015); Dapelo and Bridgeman (2018), after a small initial value of  $10^{-5}$  s, the  
 269 timestep was corrected at each iteration in order to keep the maximum Courant number near,  
 270 but less than, the limit of 0.2. Following this procedure, after the initial transient, the  
 271 timestep was observed to be between 0.0013 and 0.14 seconds.

272 At each timestep, the solution was considered as converged when the residual for the  
 273 pressure fell below  $10^{-7}$ , and for all the other quantities below  $10^{-6}$ .

274 The initial condition consisted of a system configuration with a fully-developed bubble  
 275 plume. In order to obtain this system configuration, a series of preliminary, first-order  
 276 transient PISO runs was performed for a computational time of 60 s. In these preliminary  
 277 runs, the bubble plume developed from a state with no bubble and no liquid phase motion.  
 278 Different initial conditions for  $\chi$  (“seeding”) were defined as follows:  $\chi = 0$  everywhere,  
 279 apart from small, selected portions of the domain, where  $\chi = 1$ . A more detailed discussion  
 280 on the specific seeding choices is reported below, in Section 3. The last timestep of the  
 281 preliminary runs served as the initial condition for a series of main, second-order transient  
 282 PISO runs, which was performed for an additional 1,140 s and for an overall computational  
 283 time of 1,200 s in order to replicate the mixing time reported in Table 2. As in Dapelo and  
 284 Bridgeman (2018), binary files were collected for every integer-second timestep.

285 The boundary conditions follow Dapelo and Bridgeman (2018) and are described as follows.  
 286 Top: zero constant value for pressure, free-slip for all the other fields. Wall/bottom: constant  
 287 zero for velocity, zero gradient for tracer concentration, standard wall function for turbulent  
 288 dissipation and Reynolds stress, and pressure adjusted such that the velocity flux is zero.

289 Front/back: cyclic for all the fields. The values of  $C_\mu$ ,  $\kappa$  and  $E$  for the wall functions were  
 290 set to 0.09, 0.41 and 9.8 respectively. The initial conditions for the preliminary runs were:  
 291  $4.95 \cdot 10^{-4} \text{ m}^2 \text{ s}^{-3}$  for the  $\varepsilon$  field, zero for  $p$ ,  $u$  and  $R_{ij}$ . The differencing schemes used were:  
 292 linear for interpolations, limited central differencing for the Gradient operator, linear for the  
 293 Laplacian, Van Leer for all the other spatial operators, first-order Eulerian scheme for the  
 294 time derivative in the preliminary runs and second-order backward for the main runs.

### 295 **3. Results and Discussion**

296 Four series of runs were performed under the following conditions: (i) biogas injection  
 297 through the original nozzle series at the distance  $R_1$  from the axis (labelled as “Original”);  
 298 (ii) injection through the additional series at distance  $R_2$  (“New”); (iii) switching biogas  
 299 injection from the original to the new nozzle series every minute and vice-versa, starting  
 300 from injecting from the original (“1 min switch”); and (iv) switching every five minutes (“5  
 301 min switch”).

302 The series of runs were repeated for all the rheologies reported in Table 1, and for two  
 303 different seedings, as shown in Figure 2. The small triangles on the inclined bottom  
 304 represent the location of the nozzle series.

305 [Figure 2 about here.]

306 In the seeding configuration labelled as “Seed 1”, the seeding was performed in a restricted  
 307 area near the sludge feed location in the digester, while in “Seed 2”, the seeding was  
 308 performed uniformly throughout the domain. This scenario was considered in order to  
 309 investigate both how new sludge is spread throughout the digester (“Seed 1”), and how  
 310 further mixing of pre-existing sludge occurs (“Seed 2”).

311 In Dapelo and Bridgeman (2018), it was concluded that the value of input mixing power of  
 312 the original design was excessive, and could be halved without compromising mixing  
 313 quality. Hence, the value of biogas flow rate,  $Q = Q_{\max}/2 = 2.3585 \cdot 10^{-3} \text{ m}^3 \text{ s}^{-1}$  was used in



all the computational work reported here.

### 3.1. Mesh Independence

Two grid independence tests were performed following Celik et al. (2008). The values of uniformity index and relative dead volume were computed at  $t = 300$  s for each of the grids considered in this work. The results of the tests are reported in Table 4.

[Table 4 about here.]

In all the cases apart from the relative dead volume in the Newtonian case, Grids 1, 2 and 3 fell well within the asymptotic range of convergence, while Grid 4 was found to be outside. Dapelo and Bridgeman (2018) performed a similar test on average shear rate and found that Grid 1 was outside the asymptotic range of convergence. This was attributed to the fact that bubble size was no longer negligible on the finest grid. In light of these findings and considering the need to reduce computational expense where possible, Grid 2 was chosen for the numerical work reported here.

### 3.2. Evaluation of Uniformity Index

Fig. 3 shows the value of the uniformity index over time. The quantities  $t_{0.10}$  and  $t_{0.05}$  are the times the system takes for the uniformity index to fall below 0.1 and 0.05 respectively, and can be interpreted as the times the system needs to reach a degree of mixing of 90% and 95% respectively.

[Figure 3 about here.]

The values of  $t_{0.10}$  and  $t_{0.05}$  are reported in Table 5.

[Table 5 about here.]

In the “Original” configuration, new sludge (“Seed 1”) remained close to the injection zone, with the exception of a modest displacement in the 2.5% TS case towards the end of the

simulation run. Pre-existing sludge (“Seed 2”) was spread throughout the domain, with an acceleration occurring once again in the 2.5% TS case at around the end of the run. Crucially, however, the uniformity index never fell below 0.1 in both cases, thus indicating ineffective mixing.

In the “New” configuration, a marginal improvement of the mixing conditions for new sludge was observed, when compared to the “Original”, while no significant change occurred for old sludge (“Seed 2”). However, as in the “Original” configuration, the uniformity factor did not fall below 0.1.

In the “1 min switch” configuration, a significant improvement of the mixing conditions was observed. The uniformity index dropped after around 120 s for “Seed 1” (around 60 s for “Seed 2”) and, with the exception of the Newtonian case, fell below 0.1 after 580—680 s (380—510 s), and below 0.05 after 720—870 s (510—680 s). This showed that: (i) the strategy of switching biogas injection between two nozzle series every minute was effective in improving mixing; and (ii) this strategy achieved a satisfactory level of mixing (i.e.,  $UI < 0.1$  for “Seed 1”) after approximately 600 s, which corresponded to half of the original design’s mixing time, and hence, half of the overall mixing energy determined in Dapelo and Bridgeman (2018), and one quarter of the original design’s overall mixing energy.

The “5 min switch” configuration displayed a trend similar to the “1 min switch”. However, the reduction in the uniformity factor took place at a slower rate:  $t_{0.10}$  occurred 140—190 s later than in “1 min switch” for “Seed 1” (130—180 s for “Seed 2”), while  $t_{0.05}$  was delayed by 100—170 s (100—310 s). This indicated that, despite constituting an improvement if compared to “Original” and “New” configurations, “5 min switch” was less effective than “1 min switch”.

### 3.3. Evaluation of Dead Volume

The value of the relative dead volume over time is shown in Figure 4. This value displayed significant variability, thus making it impossible to derive any evaluation of the degree of

363 mixing from it.

364 [Figure 4 about here.]

365 This behaviour may be an artefact of the way in which dead volume is defined. As discussed  
 366 in Section 2.1.2, the definition of dead volume depends on the value of the maximum  
 367 velocity. This makes the value of dead volume a function of the fluctuation of the maximum  
 368 velocity. However, Fig. 4 shows strong fluctuations of the maximum velocity in all the  
 369 simulations, throughout the whole simulated time interval, and hence, giving rise to the  
 370 strong variability of the dead volume.

371 This result shows that, despite being frequently used in the previous literature, relative dead  
 372 volume is an inappropriate criterion to assess mixing.

### 373 *3.4. Evaluation of Relative Occupancy Intervals*

374 The evolution of the relative occupancy intervals is displayed in Fig. 5.

375 [Figure 5 about here.]

376 Ten intervals, following a logarithmic scale, were chosen, as shown in the figures' legends.

377 In this way, it was possible to investigate the relative importance of different orders of  
 378 magnitude for the value of  $\chi$ —in particular, of very low concentration  $\chi < 10^{-9}$ .

379 In the “Original” configuration, “Seed 1”, the relative occupancy of very low concentrations  
 380  $\alpha_0$  remained dominant for almost the entire duration of the runs, with a marginal drop  
 381 occurring only at the end of the simulated time interval. This indicated that the mixing  
 382 mechanism was unable to spread effectively new sludge away from the injection zone.

383 In the “Seed 2” case,  $\alpha_0$  was shown to drop at the very start of the mixing time, thus  
 384 indicating that old sludge actually undertook mixing. However, coexistence of all the  
 385 intervals and failure of  $\alpha_0$  to vanish showed that mixing occurred only partially.

386 In the “New”, both “Seed 1” and “Seed 2” cases show a behaviour qualitatively similar to

the “Original, Seed 2” case. This means that new sludge is spread throughout the digester and old sludge undertakes mixing, but both only to a partial extent.

In the “1 min switch” and “5 min switch” configurations,  $\alpha_0$  dropped rapidly and vanished after a time around the corresponding  $t_{0.10}$ . At the same time, a single interval, different from  $I_0$ , became dominant. This means that mixing could be considered as complete after this time.

Finally, the evaluation of the relative occupancy intervals showed that the behaviour of the Newtonian model differed qualitatively from the non-Newtonian. This was evident from both observing the quantitative values of the uniformity index, and the qualitative behaviour of the relative occupancy intervals, in the “Original” and “New” configurations. Thus, the choice of Newtonian in place of non-Newtonian rheology altered the flow patterns, as previously noted by Wu and Chen (2008). For this reason, despite the fact that several researchers have adopted Newtonian rheology to model sludge in previous work (Vesvikar and Al-Dahhan, 2005; Karim et al., 2007; Meroney and Colorado, 2009), results shown here indicate that is approach should be avoided.

#### 4. Conclusions

The use of uniformity index is encouraged over dead volume as a quantitative mixing evaluation criterion.

Switching nozzle series every minute greatly improved mixing quality for all the rheology models, with the optimum degree of mixing being reached after 600 s from the onset of mixing.

Qualitative observations showed that the Newtonian system behaves differently from all the non-Newtonian models. Accordingly, the use of Newtonian models is discouraged.

## 410 **Supplementary Material**

411 E-supplementary data, showing more graphical details of the mesh used in this work, can be  
412 found in online version of the paper.

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423 None.

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Table 1: Rheological properties of sludge, from Dapelo and Bridgeman (2018). “ $|\dot{\gamma}|$  range” refers to the limits of the shear range interval in which the experimental measurements were performed.

	TS (%)	$\tau_0$ (Pa)	$K$ (Pa s <sup><i>n</i></sup> )	$n$ (–)	$ \dot{\gamma} $ range (s <sup>–1</sup> )
Power-law Landry et al. (2004)	2.5	0	0.042	0.710	226–702
	5.4	0	0.192	0.562	50—702
	7.5	0	0.525	0.533	11—399
Herschel-Bulkley Baudez et al. (2013)	1.85	0.092	0.169	0.308	0.01–30
Newtonian	–	0	12	1	–

Table 2: Details of the digester geometry, from Dapelo and Bridgeman (2018). Sludge feed inlet is located on a side wall, at a height  $h/4$  below the top sludge level. Courtesy of Severn Trent Water Ltd.

External diameter	$D_{\text{ext}}$	14.63 m
Diameter at the bottom of the frustum	$D_{\text{int}}$	1.09 m
Cylinder height	$h$	14 m
Frustum height	$h_0$	3.94 m
Distance of original nozzle series from axis	$R_1$	1.83 m
Distance of new nozzle series from axis	$R_2$	5.49 m
Distance of nozzles from bottom	$h_{\text{noz}}$	0.3 m
Gas flow rate per nozzle	$Q_{\text{max}}$	$4.717 \cdot 10^{-3} \text{ m}^3\text{s}^{-1}$
Mixing time		20 min in an hour

Table 3: Details of the grids. From Dapelo and Bridgeman (2018).

Id.	Number of cells	Max skewness	Max aspect ratio	Non-ortho max	Non-ortho avg	Volume min (m <sup>3</sup> )	Volume max (m <sup>3</sup> )	Vol wedge (m <sup>3</sup> )
1	394,400	1.123	13.24	30.03	14.00	1.500e-5	1.011e-3	215.8
2	98,420	1.064	9.974	30.00	13.66	3.158e-5	4.241e-3	215.8
3	36,720	1.112	10.53	30.03	13.78	3.333e-5	1.116e-2	215.3
4	18,760	1.304	13.54	30.01	13.84	4.286e-5	2.144e-2	215.3

Table 4: GCI analysis

	Uniformity Index					Relative dead volume				
	2.5 TS	5.4 TS	7.5 TS	He.Bu.	Newton	2.5 TS	5.4 TS	7.5 TS	He.Bu.	Newton
Grid 4	0.132	0.13	0.256	0.235	0.294	0.78	0.65	0.5893	0.7399	0.23
Grid 3	0.194	0.20	0.248	0.239	0.347	0.72	0.58	0.5834	0.7421	0.24
Grid 2	0.3447	0.350	0.440	0.440	0.571	0.962	0.938	0.8909	0.9024	0.25
Grid 1	0.3478230.383	0.4340	0.4454380.5954			0.944660.9523610.901470.967				0.30
$p_2$	5.479	5.201	17.88	22.03	8.534	7.375	8.709	22.26	24.13	1.920
$p_1$	16.06	6.986	14.31	14.64	9.628	10.64	13.20	13.99	4.797	0.959
GCI <sub>2<sub>43</sub></sub>	0.091	0.10	1.6e-4	2.3e-5	0.015	0.012	0.011	1.3e-5	2.1e-6	0.073
GCI <sub>2<sub>32</sub></sub>	0.20	0.21	0.0071	0.0027	0.070	0.063	0.064	0.0019	6.3e-4	0.11
GCI <sub>1<sub>32</sub></sub>	0.011	0.12	0.017	0.017	0.052	0.026	0.020	0.014	0.10	0.25
GCI <sub>1<sub>21</sub></sub>	6.6e-6	0.00432.2e-5	1.87e-5	5.8e-4	1.6e-4	4.4e-5	2.3e-5	0.011	0.34	
Asymp.20.123	0.140	2.89e-44.04e-5		0.026	0.032	0.021	2.98e-5	9.63e-60.415		
Asymp.11.006	1.092	1.046	1.013	1.041	1.125	1.015	1.013	1.072	0.484	

Table 5: Time (in s) to obtain  $UI < 0.1$  and  $UI < 0.05$ .

	Original series		New series		1 min switch		5 min switch	
$t_{0.10}$	Sd. 1	Sd. 2	Sd. 1	Sd. 2	Sd. 1	Sd. 2	Sd. 1	Sd. 2
2.5 TS	—	—	—	—	580	380	790	620
5.4 TS	—	—	—	—	580	410	930	700
7.5 TS	—	—	—	—	680	550	1,020	950
Herschel-Bulkley	—	—	—	—	680	510	910	730
Newtonian	—	—	—	—	1,030	780	1,090	980
$t_{0.05}$	Sd. 1	Sd. 2	Sd. 1	Sd. 2	Sd. 1	Sd. 2	Sd. 1	Sd. 2
2.5 TS	—	—	—	—	720	510	890	720
5.4 TS	—	—	—	—	740	550	1,100	910
7.5 TS	—	—	—	—	850	730	1,180	1,150
Herschel-Bulkley	—	—	—	—	870	680	1,090	1,040
Newtonian	—	—	—	—	—	1,080	—	1,120

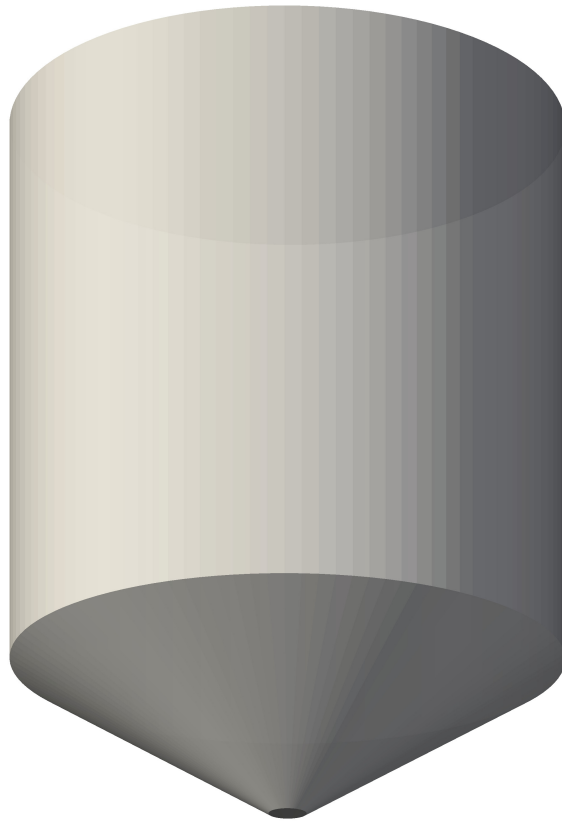


Figure 1: Computational domain. Illustrative view, from Dapelo and Bridgeman (2018).



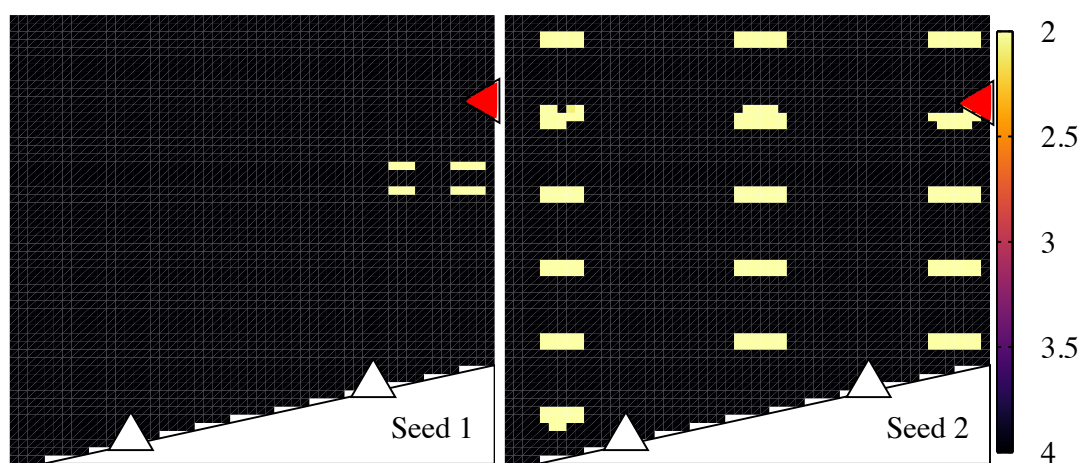


Figure 2: Seeding. Tracer concentration, logarithmic scale. The white triangles indicate where biogas injection occurred; the red triangles indicate sludge feed location.

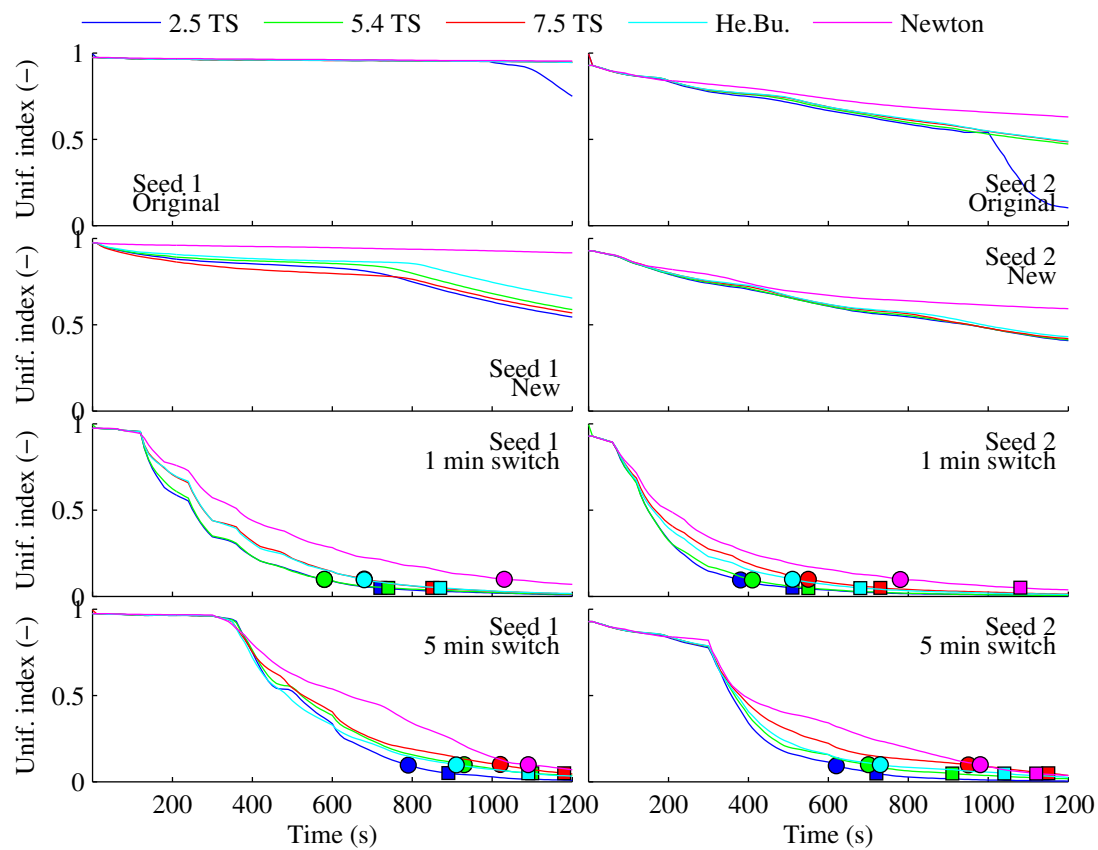


Figure 3: Uniformity index. Uniformity index over time for all the rheological models.  $t_{0.10}$  and  $t_{0.05}$  are marked with a circle and a square respectively.

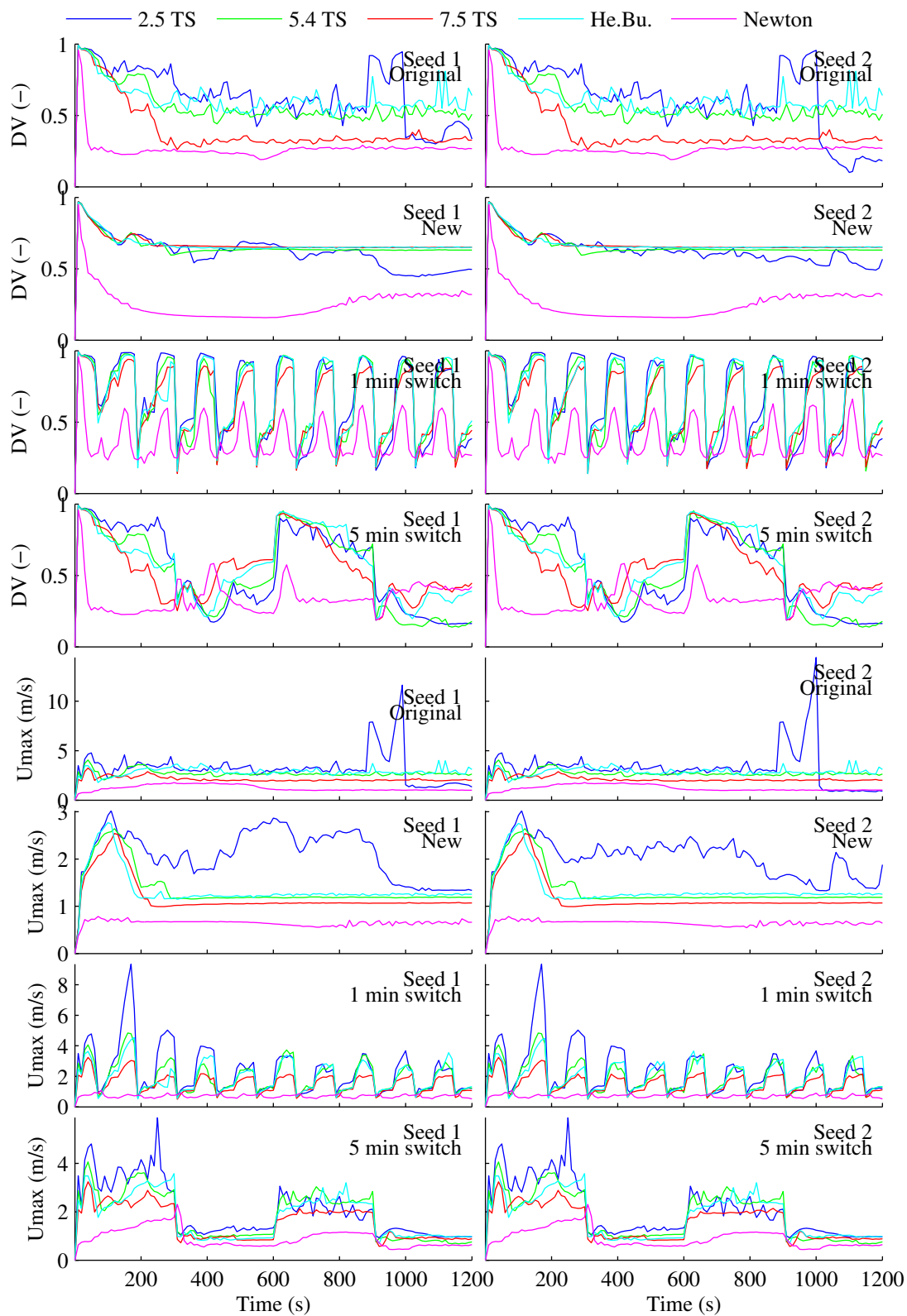


Figure 4: Dead volume. Relative dead volume and maximum velocity over time for all the rheological models.

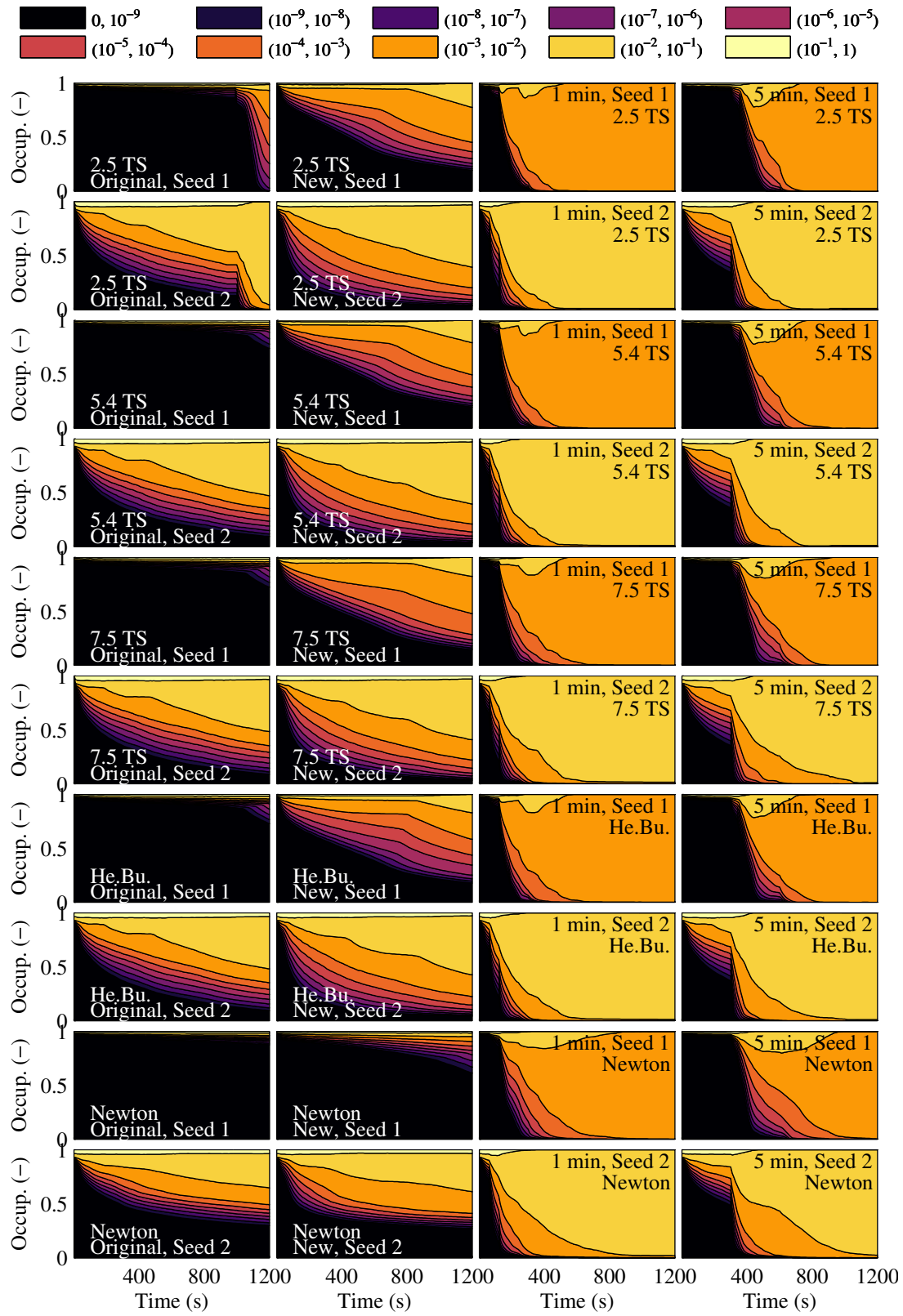


Figure 5: Relative occupancy. Relative occupancy intervals over time for all the rheological models.